

July 9, 2002

Ms. Patricia Messenger
Technical Contact
American Chemistry Council
Ethylbenzene HPV Task Group
1300 Wilson Boulevard
Arlington, VA 22209

Dear Ms. Messenger:

The Office of Pollution and Toxics is transmitting EPA's comments on the robust summaries and test plan for Diethylbenzene-Rich Streams, posted on the ChemRTK HPV Challenge Program Web site on December 12, 2001. I commend The American Chemistry Council Ethylbenzene HPV Task Group for its commitment to the HPV Challenge Program.

EPA reviews test plans and robust summaries to determine whether the reported data and test plans will provide the data necessary to adequately characterize each SIDS endpoint. On its Challenge Web site, EPA has provided guidance for determining the adequacy of data and preparing test plans used to prioritize chemicals for further work.

EPA will post this letter and the enclosed Comments on the HPV Challenge Web site within the next few days. As noted in the comments, we ask that The American Chemistry Council Ethylbenzene HPV Task Group advise the Agency, within 60 days of this posting on the Web site, of any modifications to its submission.

If you have any questions about this response, please contact Richard Hefter, Chief of the HPV Chemicals Branch, at 202-564-7649. Submit questions about the HPV Challenge Program through the HPV Challenge Program Web site "Submit Technical Questions" button or through the TSCA Assistance Information Service (TSCA Hotline) at (202) 554-1404. The TSCA Hotline can also be reached by e-mail at tsca-hotline@epa.gov.

I thank you for your submission and look forward to your continued participation in the HPV Challenge Program.

Sincerely,

Oscar Hernandez, Director
Risk Assessment Division

Enclosure

cc: W. Sanders
A. Abramson
C. Auer
M. E. Weber

**EPA Comments on Chemical RTK HPV Challenge Submission:
Diethylbenzene-Rich Streams Category**

SUMMARY OF EPA COMMENTS

The sponsor, the American Chemistry Council Ethylbenzene Panel HPV Task Group, submitted a test plan and robust summaries to EPA for the "Diethylbenzene-Rich Streams Category" dated October 26, 2001. EPA posted the submission on the ChemRTK HPV Challenge Web site on December 12, 2001. The diethylbenzene-rich streams category is identified by CAS numbers 68608-82-2 (by-products from ethylenated benzene) and 25340-17-4 (diethylbenzenes).

EPA has reviewed this submission and has reached the following conclusions:

1. Category Definition and Justification. EPA is unclear whether the products discussed in the test plan constitute a category. They appear to define a mixture that varies rather narrowly depending on manufacturer and process conditions and that is adequately defined by CAS No. 25340-17-4 (diethylbenzenes). The definition of CAS No. 68608-82-2 is very broad and does not appear to be addressed by the test plan. The submitter needs to explain how substances defined by CAS No. 68608-82-2 could be adequately represented by the substance described in this test plan.
2. Test Substance. The submitter needs to address issues of test substance composition for existing and planned studies.
3. Physicochemical and Environmental Fate Data. The submitter indicates in its test plan table (page 9) that adequate biodegradation data exist for CAS No. 25340-17-4 and CAS No. 68608-82-2. However, the submitter provided a robust summary only for CAS No. 25340-17-4. The submitter needs to provide a robust summary for CAS No. 68608-82-2, or clarify this discrepancy.
4. Health Effects. Adequate testing on all SIDS-level health effects endpoints have been conducted on "mixed diethylbenzene stream." However, the submitter needs to provide the composition of the tested mixture and/or needs to confirm that the substances used in these tests are similar in composition to analyzed samples of diethylbenzene-rich streams. In addition, the submitter needs to address deficiencies in the robust summaries.
5. Ecological Effects. All data for ecotoxicity endpoints are inadequate. All the studies were performed in static conditions with nominal concentrations in which the chemical's volatility during the test was not addressed. In addition, the submitter needs to provide the robust summaries for the data discussed in the test plan for the acute and chronic ecotoxicity of 1,4-diethylbenzene.

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.

**EPA COMMENTS ON DIETHYLBENZENE-RICH STREAMS
CATEGORY CHALLENGE SUBMISSION**

Category Definition

The submitter defined diethylbenzene-rich streams as a category consisting of streams that contain "a predominance of diethylbenzene isomers and are produced during ethylbenzene manufacture." The submitter stated that diethylbenzene-rich streams are identified by two CAS registry numbers: 25340-17-4, diethylbenzene (also known as "mixed diethylbenzenes"), and 68608-82-2, by-products from ethylenated

benzene (also known as “polyethylbenzenes”).

The submitter summarized composition data of samples from four companies of their diethylbenzene-rich streams. Diethylbenzene isomers represented 87.6 to 98.8% of the weight of these samples.

Alkylbenzenes accounted for 1-5% of the weight, and other components were <0.1% each. Thus, this substance can reasonably be characterized as “diethylbenzenes” and assigned CAS No. 25340-17-4.

However, the TSCA Inventory definition of CAS No. 68608-82-2 is “[a] complex combination of hydrocarbons obtained by the alkylation of benzene with ethene. It consists primarily of ethylbiphenyls, diethylbenzenes with lesser amounts of butylbenzenes and polyethylbenzenes.” The substance discussed by the submitter does not seem to fit this definition. The test plan refers just once to separation into a diethylbenzene-rich stream and a bottoms stream; the latter would seem most likely to fit the definition of CAS No. 68608-82-2, and intuitively would not resemble the diethylbenzene stream in composition. The submission leaves this point unclear because it did not provide separate analytical data for the diethylbenzene-rich and bottoms streams.

The information provided does not allow EPA to agree with the submitter that the ranges of composition for streams corresponding to CAS No. 25340-17-4 and CAS No. 68608-82-2 “are very similar.” The data do not show that the composition of CAS No. 68608-82-2 is “similar” to CAS No. 25340-17-4, but rather that only the latter CAS number reasonably describes the samples analyzed.

Category Justification

As indicated by EPA’s comments above, it is not clear whether diethylbenzene-rich streams constitute a category. The test plan describes a mixture that varies in composition across manufacturers, depending on the starting materials, reactor conditions, and post-reactor processing conditions. As noted above, the description of the stream is narrower than the definition of CAS No. 68608-82-2, but appears to fit CAS No. 25340-17-4. Therefore, the submitter needs to justify why CAS No. 68608-82-2 is adequately represented by the diethylbenzene-rich streams described in this test plan or submit a separate test plan for CAS No. 68608-82-2.

Test Plan

Test Substance.

Because of the questions raised above under “Category Definition,” the submitter needs to confirm, for example by providing analytical data, that the composition of the test substance used in each existing study is similar to that of the analyzed diethylbenzene-rich streams given in the test plan. Further, the submitter states on page “i” of the test plan that “samples of streams will be combined to form a test sample for testing.” If existing studies were done on combined streams, it is important to include this information in the robust summary.

Finally, to help justify inclusion of CAS No. 68608-82-2 in the test plan, the submitter needs to show that the proposed test substance represents both the proposed CAS numbers.

Chemistry (melting a point, boiling point, vapor pressure, water solubility, and partition coefficient).

For physical chemical properties, the submitter needs to provide measured values. In particular, boiling points (decomposition points if appropriate), water solubilities, and vapor pressures should be measured unless precluded by experimental obstacles. The use of estimated values introduces uncertainties that then become magnified in modeling applications. A measured value for water solubility is especially

important because it can help determine the need for aquatic toxicity testing of more hydrophobic chemicals.

Environmental Fate (photodegradation, stability in water, biodegradation, transport/distribution).

The submitter's approaches to photodegradation and stability in water endpoints are acceptable for the purposes of the HPV Challenge Program.

Biodegradation.

The test plan (page 9) indicates that adequate biodegradation information is available for CAS No. 25340-17-4 and CAS No. 68608-82-2. However, in the robust summaries, the submitter provides biodegradation data for only CAS No. 25340-17-4. The submitter needs to address this discrepancy.

Transport and Distribution.

The submitter's approach to this endpoint is acceptable for the purposes of the HPV Challenge Program. However, EPA recommends that the submitter conduct its transport and distribution modeling using the fugacity model level III. When developing the fugacity model, the sponsor needs to provide the assumptions and data inputs to the model (see Guidance for Robust Summary Preparation). Furthermore, the submitter should use measured physicochemical data as inputs into its transport and distribution model. The use of estimated values introduces uncertainties that then become magnified in modeling applications. EPA prefers using the EQC Level III model from the Canadian Environment Modeling Centre at Trent University because it provides a more rigorous level of analysis. This model can be found at the following Web address: <http://www.trentu.ca/academic/aminss/envmodel/>.

Health Effects (acute toxicity, repeated-dose toxicity, genetic toxicity, and reproductive and developmental toxicity).

Although the submitter provided adequate data for all health effects SIDS-level endpoints, EPA will determine their relevancy after the submitter provides confirmation that the composition of test substances used in the studies is similar to that of the analyzed diethylbenzene-rich streams stated in the test plan. The submitter also needs to address the specific deficiencies in the robust summaries.

Ecological Effects.

The sponsor proposed no additional ecotoxicity testing; however, available ecotoxicity data are inadequate for all endpoints because the studies were performed in open systems without measured concentrations. The submitter needs to conduct all ecotoxicity endpoints in closed system testing, or with measured concentrations.

The submitter needs to provide robust summaries for 1,4-diethylbenzene as these data are discussed in the test plan (page 4).

Specific Comments on the Robust Summaries

Health Effects.

For all robust summaries of studies in which the test substance was referred to as "mixed diethylbenzene stream," the submitter needs to confirm that the composition of the test substances is similar to that in the test plan.

Acute oral toxicity. In the Biodynamics, Inc. (1987) study, the submitter needs to provide mortality, clinical signs, and gross pathology data by dose and sex.

Genetic toxicity.

Reverse mutation in bacteria. For the Chevron (1991) assay in *Salmonella*, missing information includes the concentrations at which the number of revertants was significantly increased.

Micronucleus assay in vivo. Missing information includes the method for staining the cells, and the number of cells evaluated per animal/dose.

Reproductive Toxicity.

Inhalation exposure. Missing information includes the method of generating the test atmosphere.

Oral exposure (1,4-diethylbenzene study). There is a discrepancy between the test type "Inhalation" and the route of administration "Oral gavage" in the robust summary.

Ecotoxicity.

Robust summaries were submitted for acute studies on "mixed diethylbenzene stream" in fish, invertebrates, and aquatic plants. However, the submitted studies were inadequate on all ecotoxicity endpoints. The robust summary for all future ecotoxicity studies should follow the "Guidance on Developing Robust Summaries" at <http://www.epa.gov/opptintr/chemrtk/guidocs.htm>.

Followup Activity.

EPA requests that the submitter advise the Agency within 60 days of any modifications to its submission.